DOCUMENT RESUME

ED 116 610 IR 002 476

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|---|---|
| AUTHOR | Masten, F. A.; And Others |
| TITLE | Computer Augmented Lectures (CAL): A New Teaching Technique for Chemistry. |
| INSTITUTION | Texas Univ., Austin. Project C-BE. |
| SPONS AGENCY | National Science Foundation, Washington, D.C. |
| REPORT NO | EP-15-7-10-73 |
| PUB DATE | 10 Jul 73 |
| NOTE | 25p.; For related documents see IR 002 463 and 464 |
| EDRS PRICE | MF-$0.76 HC-$1.58 Plus Postage |
| DESCRIPTORS | Chemistry Instruction; *College Instruction; *Computer Assisted Instruction; Costs; Input Output Devices; *Lecture; *Multimedia Instruction; On Line Systems; Performance Specifications; Program Descriptions; Program Evaluation; Projection Equipment; Teaching Methods; *Video Equipment |
| IDENTIFIERS | Computer Augmented Lectures; *Project C BE; University of Texas Austin |

ABSTRACT

A new technique described as computer augmented lectures (CAL) is being used at the University of Texas at Austin. It involves the integration of on-line, interactive, time sharing computer terminals and theater size video projectors for large screen display. This paper covers the basic concept, pedagogical techniques, experiments conducted, technical hardware specifications, programing languages used, and the economics involved. (Author/E1H)

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ED116610

# COMPUTER AUGMENTED LECTURES (CAL):

# A NEW TEACHING TECHNIQUE FOR CHEMISTRY

EP-15/7/10/73

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IR 002 476

This study was supported in part by Project C-BE under Grant GY-9340 "The Use of Computer-Based Teaching Techniques in Undergraduate Science and Engineering Education" from the National Science Foundation to the University of Texas, Drs. John J. Allan and J. J. Lagowski, Co-Directors.

# COMPUTER AUGMENTED LECTURES (CAL): A NEW TEACHING TECHNIQUE FOR CHEMISTRY


## ABSTRACT

A new technique described as computer augmented lectures (CAL) is being used at The University of Texas at Austin. It involves the integration of on-line interactive time-sharing computer terminals and theatre size video projectors for large screen display. This paper covers the basic concept, pedagogical techniques, experiments conducted, technical hardware specifications, programming languages used, and the economics involved.

# COMPUTER AUGMENTED LECTURES (CAL):

# A NEW TEACHING TECHNIQUE FOR CHEMISTRY

## INTRODUCTION

In the last several years, computer learning techniques have been widely applied, primarily to individual student interaction with a teaching program. Such computer assisted instruction (CAI) has provided a way to allow students to learn at their own rate independent of the average students' ability. Unfortunately, CAI is very expensive both in terms of hardware (paper, teletypes, etc.) and in terms of computer usage. Logistically, the problem of scheduling teletype use is quite difficult. Also, since flexibility in CAI requires sophisticated program branching, CAI programs are very complex and, consequently, not easily transferred between schools. While such individualized instruction with highly flexible programs on high speed computers is indeed useful, there would also seem to exist a demand for applying the computational power of standard computers to teaching situations in a more economical and transferrable way. CAL provides such a way. Before describing the application, computer augmented lectures (CAL) must be defined. CAL is a method for using interactive commonly supported computer programs for integration into a video projection system to display information before large numbers of students for the purpose of enhancing learning.

The following section contains a detailed description of CAL instructional modes as used experimentally at The University of Texas at Austin.

## INSTRUCTIONAL MODES OF CAL

CAL was used in two different modes, an introductory tutorial mode and a compute mode. The tutorial mode employed a scenario similar to conventional CAI, but with the advantage of the instructor's presence for explanation. This mode was used to provide a step-by-step introduction to a subject, illustrating it with several simple examples. Through the tutorial numerous holds were provided so that considerable time might be spent explaining the steps in the problem. After several tutorials had been completed and the basic steps mastered, it was switched to the compute mode. Here input and output were reduced to a minimum and the full computational powers of the computer were utilized to treat quickly a large number of problems of the same general type but of varying complexity. The entire range of applicability of the theory may be investigated by immediate exact calculation. An

outstanding feature is CAL's ability to respond almost immediately to questions posed by the students. Both of the above modes can be used either (1) on line interactively via data sets and telephone lines, or (2) passively when the computer is not available. The latter is accomplished by prerecording the computer program on an ordinary inexpensive cassette recorder. The play-back recorder transmits the recorded data signals into the data set connector wired for private line use. This latter technique is described in detail in the technical section (Appendix I).

## EXPERIENCES USING CAL

Early efforts using CAL were confined primarily to the area of chemistry. CAL was used to assist in the teaching of modern theories of chemistry. These topics are usually omitted in introductory courses, but nevertheless form a large part of modern chemical research. For this reason, over the past seven years a freshman course has been offered entitled "The Vector Space Theory of Matter" (VSTM) to above average students at The University of Texas at Austin. Because of the success of the technique in presenting these topics, it is being applied to the standard large sections of general chemistry. In the Fall semester, 1972, the elements of Hückel molecular orbital theory was taught in the general chemistry course of 250 students using CAL. The students saw the application of modern theory to problems in chemistry without becoming bogged down in mathematical detail. Appendix III shows a sample output from the Hückel tutorial for the cyclopropenyl radical and the compute mode for azulene. (A colon is inserted to indicate a pause for class discussion.) Figure 2 illustrates Bill Seitz demonstrating the Hückel Matrix. After two computer augmented lectures, a student commented that "this stuff is sure a lot easier than pH." In the last class meeting, a review of pH and titration using CAL was presented. In forty-five minutes it was possible to computer and display titration curves for strong acid-strong base, weak acid-strong base, and di-protic acid-strong base, for arbitrary dissociation constants and initial concentrations, thus reviewing without extensive computation many important concepts.

The attendant flexibility for module use in classes with widely differing aptitudes and backgrounds has resulted in our use of the Hückel module for both a freshman chemistry class and an NSF summer short course for college and university chemistry teachers.

While CAL was developed for courses in chemistry, the technique is applicable to other subjects. Currently applications to introductory physics are being investigated at the University of Texas by Professor J. D. Gavenda, Department of Physics. In addition, courses in business, statistics, or computer science could also benefit from CAL.

## JUSTIFICATION FOR USING CAL

The principal reasons for using CAL can be summarized as follows:

1. A low hardware cost per student--by requiring only one remote terminal for large numbers of students, CAL shares the cost per student, both for hardware and computer time in the most economical way possible.

2. Simplicity in programming--because of the live instructor interface between the students and the computer, the program does not require internal loops to correct input errors. Instructors are especially good at this.

3. Interrupt capability--the instructor may interrupt the program at any time to interpret and explain points raised by the students.

4. Transferability--because each module (or program) is in itself separate and complete, and since the common software imbedded programs are also very simple, CAL modules are easily transferrable from one college to another. In addition, the modest hardware requirement permits use of CAL at schools where a large number of remote terminals are not available.

5. Good interactive capabilities--once the logistics have been established, problems may be submitted and formulated from the floor. "What if" questions can be answered quickly and completely.

6. Compute power--as a consequence of the speed of machine calculations, many related problems may be solved during a single lecture, so that the student acquires quickly a wide range of experience, operational understanding and even intuition. One can thus illustrate rather than merely assert the generality of the procedure being presented.

7. Permanent storage recordability--the display for each lecture or problem can be permanently recorded for playback on cassette magnet tape, punched paper tape, or video tape, providing for (a) backup in the event of computer failure during lecture, (b) opportunity for review by individual students, and (c) transferability of the lecture to other colleges.

8. Standardization--it can standardize the general approach among different lecture sections of the same course.

9. Superior display--the instructor is released from the blackboard, making it easier to communicate with the class.

10. Dynamic presentation--the student's attention is focused on the projected material because of something like the "follow the bouncing ball" syndrome.

11. Flexibility--since each module is independent, any course may use those which are most appropriate, and in any order.

12. Utilization of instructor personality--the instructor retains control of the classroom situation. He can teach at a rate compatible with student capabilities and inject his own personal experiences and humor into the lecture. Unlike most computer learning techniques, the computer in CAL assists rather than replaces the teacher. ( A word of caution is advised in using the above techniques. Once the instructor makes a point before the class, it is best to erase or clear the screen. If this is not done, the student's attention is drawn away from the lecturer to the screen. )

13. Monetarily and logistically, the obvious advantages of replacing 250 individual interactions with a single CAL lecture cannot be overemphasized.

14. CAL programs are vastly simpler than CAI since all branching for explanation is done by the instructor, thus releasing the computer for the job of computing. FORTRAN IV was used as the programming language, and through its commonality and simplicity, permits easy transfer of all CAL modules.

With the increase in demands put on current computer facilities, the advantages stated above should become more important.

## PEDAGOGICAL ASPECTS

CAL has several teaching advantages, one such attribute being the ability to program real time linear development of lecture material, which has long been recognized as the advantage of conventional blackboard use over slides. CAL maintains a real time relationship to the ideas being presented, thus releasing the instructor from the blackboard and improving the clarity and accuracy of the lecture. Also, the flexibility of CAL for immediate response to student questions cannot be obtained via film or slide display. The use of a cassette or punched tape recording can also provide an instant replay capability for student review without group presentation. An additional flexibility also is provided by CAL by the immediate compute-power available, which can extend ordinary lecture material into new, more complicated situations, as was discussed earlier. Finally, the flexibility of CAL due to instructor's teaching style and personality permits a variety of learning experiences. In contrast to computer assisted instruction, or even video display of CAI output, CAL requires only the computer-power and the nucleus for a lecture instead of a rigidly locked in single teaching pace and method.

## ECONOMICS OF CAL

The economics of using one terminal with associate data set and one video projector for a group of up to 300 students averages out to less than five cents per student/ per hour/ per lecture. This is calculated on the basis of an amortization period of five years for the video projector and terminal, central processor costs, communications costs, personnel costs and maintenance costs, divided by the total number of student hours per year multiplied by five years.

The calculations used to derive the above costs are as follows:

Major Equipment Items:

| | | | | |
|---|---|---|---|---|
| Videoprojector | $11,000 | | | |
| Cathode Ray Tube Terminal | 2,100 | | | |
| Acoustic Coupler | 300 | | | |
| TOTAL | $13,400 | - | 60 months | = $223.33/mo |

| | | | |
|---|---|---|---|
| Communication Costs: | Telephone @ $12.50/mo. | = | $12.50 / mo. |
| Central Processor Time: | 1 TM hour/mo. | = | 52.00 / mo. |
| Computer Communications: | 60 hours/mo. x $.40 hr. | = | 24.00 / mo. |
| TOTAL: | | | $88.50 / mo. |

| | | |
|---|---|---|
| Major Equipment Items | = | $223.33 / mo. |
| Maintenance | = | 95.00 / mo. |
| Personnel (½-time Grad Student) | = | 400.00 / mo. |
| Communication Costs, CPU Time, and Computer Communications | = | 88.50 / mo. |
| TOTAL: | | $806.83 / mo. |

Assume 15 lecture hours/week or 60 hours/mo./300 students:

$$\frac{\$806.83/\text{mo.}}{60} = \$13.44/\text{hr.}$$

$$\frac{\$13.44}{300 \text{ students}} = \$.045/\text{hr./student}$$

## TECHNICAL PROBLEMS

Although the results of the early efforts demonstrated the feasibility of using this technique, there were many operating difficulties due to technical limitations of the 1960 vintage video equipment. Video resolution and brightness were marginal in that the video projector was primarily designed for projecting videocast images and not for displaying a full screen of computer generated alpha-numeric characters. The second problem was a local one, and was the size of the projected letters (within the screen image) with regard to both sharpness and brightness. Tests made at that time revealed that when one full line containing 80 characters was projected, most of the students at the rear of the auditorium (some 60 feet from the screen) could not read the small size letters of the text. The reason for this was that the other related equipment in this facility, being multi-purpose, could not be moved; thus, the image of the videoprojector was limited to 6 feet x 8 feet in size. This resulted in our trying to lower the lighting levels (using theatre dimmers) to a suitable level to attempt to improve resolution of the characters by increasing the contrast while still allowing enough lighting for student note-taking. Eventually it was decided to purchase a new unit that possessed the high resolution, brightness, and contrast characteristics to clearly project a 9' x 12' image. This was accomplished in January, 1973, and the unit became operational during the Spring semester of 1973. The technical specifications are shown in Appendix II.

## EVALUATION OF CAL BY STUDENTS

Following the completion of the course in theoretical chemistry, an evaluation of student reaction to CAL was made using a questionnaire form. The most frequent complaints concerning CAL were: (1) poor video projection clarity; (2) display presentation speed by instructor too rapid; and (3) room darkness adjustment too low. All of these problems have presently been solved. A high resolution rear screen projector is now being employed, which has good clarity, and can be operated with room lights on as shown in the figure. In addition, the data transmission rates used for display of characters on the cathode ray tube display has been slowed down from 30 characters to 10 characters per second in order that the student could easily

follow the interaction. A list of equipment used in this experiment is located in Table 2. With respect to teaching the Huckel theory by CAL, the student response was 100% favorable, indicating both their interest in and ability to learn modern chemical theory. CAL has thus provided access to this important area of chemistry by overcoming the mathematical and computation constraints and allowing the instructor to concentrate on methods and concepts. An artist's drawing of the terminal and video projector installation in the Academic Center Auditorium is shown in Figure 1. The listing of all of the modules (computer programs) developed for use with theoretical chemistry is contained in Table 1.

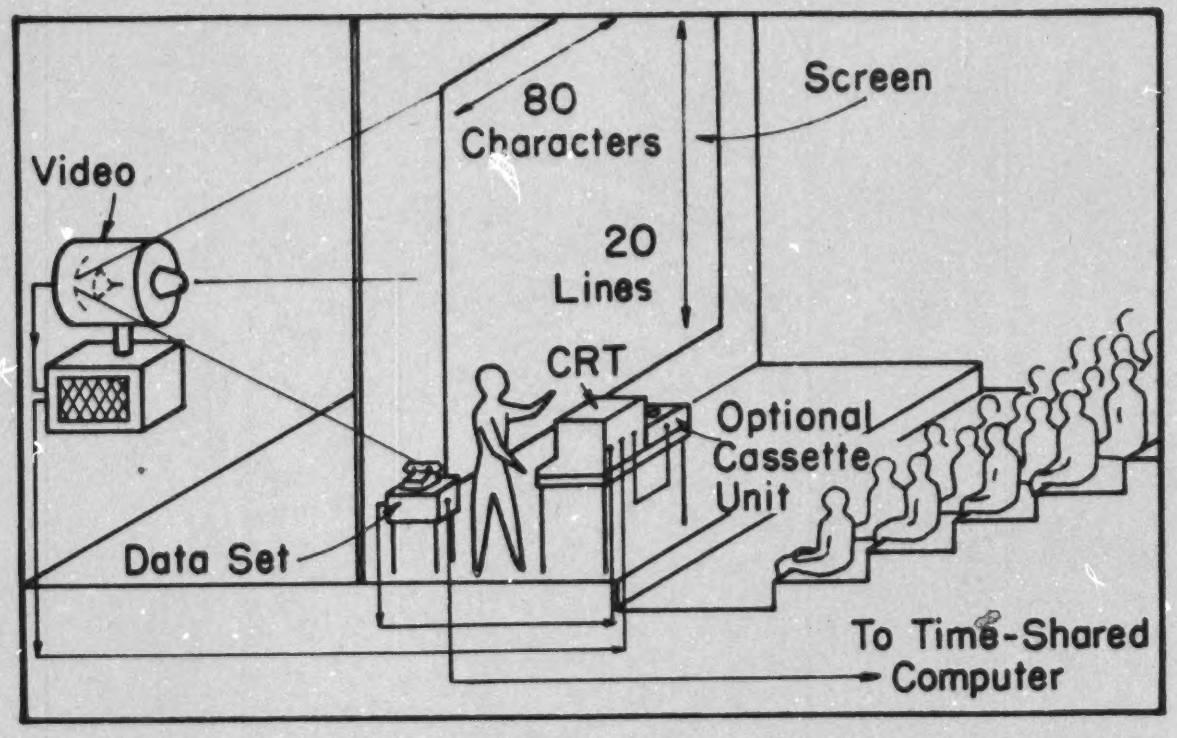


FIGURE 1

SCHEMATIC REPRESENTATION
OF A TYPICAL CAL INSTALLATION

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Miller, J. L., "Rear Projection Screens: A Designer's View," Information Display, Vol. 9, No. 3, May/June, 1972.

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TABLE 1

LIST OF COMPUTER PROGRAMS USED

IN THEORETICAL CHEMISTRY

1. Atomic Theory*
2. Hückel Theory*
3. Crystal Field Theory*
4. Nuclear Magnetic Resonance*
5. Electron Spin Resonance
6. Vibrational and Rotational Spectroscopy
7. Fine Structure
8. Nuclear Theory
9. Related Mathematical Tutorials, including
   a. Determinants
   b. Eigenvalue-Eigenvector Computation*
10. pH* (4 modules)
11. Titration*
12. Kinetics
13. Equilibrium Calculation

The table above lists the CAL modules currently in use or under development. Modules in operation are marked with an asterisk.

TABLE 2

LIST OF EQUIPMENT

Videoprojector

One (1) Amphicon Model 260A with type 22X face place (16' from projector to screen) specified for 9' x 12' projected image.

Terminal Devices

One (1) Beehive Model 1 alpha-numeric CRT fitted with standard 525 line video output BNC connector and selectable data transmission rates of 110 BPS to 2400 BPS. CRT settings use full duplex mode.

One (1) Coaxial Cable RG-59/U with BNC connectors.

One (1) Techtran Model 4100 Digital data cassette recorder with selectable data rates of 110 BPS, 300 BPS, and 1200 BPS.

Data Set

Omnitec Model 701A Acoustic Coupler

Communications

Either one (1) private (leased) line from computer to line receptacle of Acoustic Coupler using half duplex mode for transmission, or one (1) dial up line to computer using half duplex mode for transmission.

Appendix I

TECHNIQUES IN "ON-LINE"

DIGITAL CASSETTE RECORDINGS

## DESCRIPTION OF TECHNIQUE USED IN MAKING "ON-LINE" (DIGITAL CASSETTE) RECORDINGS OF INTERACTIVE COMPUTER PROGRAMS

The technique used at The University of Texas at Austin for making digital cassette recordings utilized a Techtran Corporation Model 4100 Digital Cassette Recorder. The Techtran was connected in parallel to a Beehive Model I Cathode Ray Tube Terminal. Both units were tied in to an Omnitec Model 701A Acoustic Coupler for on-line operation. The programs were recorded at 110 BPS in ASCII code on a Sony low noise digital cassette. Data switch settings were: full duplex on the CRT and half duplex on the acoustic coupler. The digital tape cassette capacity was 70,000 ASCII characters maximum. The programs could be used either on line or off line.

## Appendix II

## SPECIFICATIONS FOR VIDEO PROJECTION SYSTEM

## Appendix II

## SPECIFICATIONS FOR VIDEO PROJECTION SYSTEM

A. A high resolution cathode ray tube of 1000 lines or better.

B. A video projector (1) with the capability of projecting a full 9 x 12 foot screen image (using rear view projection) with a screen brightness of up to 15 foot lamberts in a normally lighted auditorium, (2) that would project a standard 525 line raster scan CRT output of 80 characters per line and 16 lines in a uniformly crisp and sharp image over the entire field (front view projection), (3) that was capable of plotting vector graphics type displays (1024 x 1024 resolution) through the use of a common interface device (scan converters, etc.) and common communication interface, i.e., an E.I.A. RS-232/c, (4) that could handle low, medium, and high data input rates for complex real time graphic displays, and (5) that projected in monochrome.

C. A wide band video amplifier (27 MHz).

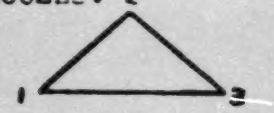
## Appendix III

## COMPUTER AUGMENTED LECTURE

## OUTPUT FOR HUCKEL THEORY

VECTOR SPACE THEORY OF MATTER: HUCKEL THEORY

HUCKEL THEORY MAKES PREDICTIONS OF SPECTRA,
REACTIVITY, IONIZATION POTENTIALS, ELECTRON AFFINITIES,
AND RESONANCE ENERGIES OF UNSATURATED ORGANIC MOLECULES.
WHAT COMPOUND SHALL WE DO?
:CYCLOPROPENYL
WE PROCEED VIA THE SIX STEP WAY.




STEP 1: SIGMA FRAME (HAMILTONIAN SELECTION)
:

A) DRAW THE STRUCTURE DIAGRAM WITHOUT HYDROGEN ATOMS.
:

B) REMOVE THE SECOND BOND IN ALL DOUBLE BONDS.
:

C) REPLACE ALL CARBON ATOMS WHICH WERE EITHER DOUBLE BONDED OR ASSOCIATED WITH A PLUS, MINUS, OR DOT SUPERSCRIPT, WITH A PLUS SIGN.
:

D) NUMBER THE CATIONS.
:

E) COUNT THE NUMBER, M, OF CATIONS.
:

ENTER THE NUMBER OF CATIONS, M, IN COLUMN 1.
:3

STEP 2: VECTOR SPACE SELECTION

V:[ [P:1>, [P:2>, [P:3> ]
:

STEP 3: HAMILTONIAN MATRIX

[H] = [ <I]H[J> ] I,J=1, 3

THIS IS A 3 X 3 MATRIX
:

PLACE AN "ALPHA" IN EACH ELEMENT ON THE DIAGONAL.
:

ALPHA
ALPHA
ALPHA

```
 FOR THE FOLLOWING QUESTIONS, DESIGNATE THE
NUMBERS OF THE APPROPRIATE CATIONS WITHOUT
DECIMAL POINTS OR SPACES.

DESIGNATE THE CATIONS SIGMA BONDED TO CATION 1
?23
THEREFORE YOU PUT A "BETA" IN FOR THE
FOLLOWING ELEMENTS:
    (1,2)
    (1,3)

DESIGNATE THE CATIONS SIGMA BONDED TO CATION 2
?13
THEREFORE YOU PUT A "BETA" IN FOR THE
FOLLOWING ELEMENTS:
    (2,1)
    (2,3)

DESIGNATE THE CATIONS SIGMA BONDED TO CATION 3
?12
THEREFORE YOU PUT A "BETA" IN FOR THE
FOLLOWING ELEMENTS:
    (3,1)
    (3,2)


              HAMILTONIAN MATRIX

?
   ALPHA     BETA      BETA
   BETA      ALPHA     BETA
   BETA      BETA      ALPHA


THE SECULAR EQUATION IS

?
        ALPHA-Y   BETA      BETA
 DET    BETA      ALPHA-Y   BETA      = 0
        BETA      BETA      ALPHA-Y
?


EIGENVALUES IN DESCENDING ORDER
?
    E(3)= ALPHA + ( -1.0000000E+00 BETA )
    E(2)= ALPHA + ( -1.0000000E+00 BETA )
    E(1)= ALPHA + (  2.0000000E+00 BETA )
?


ORBITAL ENERGY LEVEL DIAGRAM

E(2)---------    ----------E(3)


        ---------------E(1)
?
```

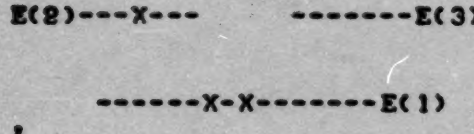
ELECTRON CONFIGURATION AND ENERGY

NEUTRAL MOLECULE N=3  N IS THE NUMBER OF ELECTRONS.

GROUND STATE

1(2) 2(1)

3 ALPHA + ( 3.0000000E+00 BETA )




FIRST EXCITED STATE

1(1) 2(2)

3 ALPHA + ( 2.4158453E-13 BETA )

CATION

1(2)

2 ALPHA + ( 4.0000000E+00 BETA )

ANION

1(2) 2(2)

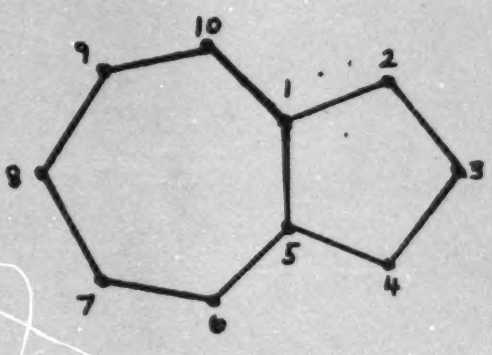
4 ALPHA + ( 2.0000000E+00 BETA )

```
IONIZATION POTENTIAL

     -1 ALPHA + (   1.0000000E+00 BETA )
!

ELECTRON AFFINITY

     -1 ALPHA + (   1.0000000E+00 BETA )
!

EIGENVECTORS

 EIGENVECTOR 3=      0.00000      -.70711       .70711

 EIGENVECTOR 2=       .81650      -.40825      -.40825

 EIGENVECTOR 1=      -.57735      -.57735      -.57735
!

   PI ELECTRON DENSITIES
      ATOM NUMBER    1       CHARGE DENSITY     1.00000E+00
      ATOM NUMBER    2       CHARGE DENSITY     1.00000E+00
      ATOM NUMBER    3       CHARGE DENSITY     1.00000E+00
!

PI BOND ORDERS
  BETWEEN ATOMS    1 AND    2
    PI BOND ORDER IS          5.00000E-01
  BETWEEN ATOMS    1 AND    3
    PI BOND ORDER IS          5.00000E-01
  BETWEEN ATOMS    2 AND    3
    PI BOND ORDER IS          5.00000E-01

***END OF TUTORIAL***
```

VECTOR SPACE THEORY OF MATTER: COMPUTE MODE

ENTER THE NUMBER OF CATIONS.
:10
NUMBER OF CATIONS IN SIGMA FRAME 10
FOR THE FOLLOWING QUESTIONS, LIST THE NUMBERS OF THE APPROPRIATE CATIONS WITHOUT DECIMAL POINTS AND WITH AT LEAST ONE SPACE BETWEEN NUMBERS. END LIST WITH A ZERO.

LIST THE CATIONS SIGMA BONDED TO CATION 1
:2 5 10 0
LIST THE CATIONS SIGMA BONDED TO CATION 2
:1 3 0
LIST THE CATIONS SIGMA BONDED TO CATION 3
:2 4 0
LIST THE CATIONS SIGMA BONDED TO CATION 4
:3 5 0
LIST THE CATIONS SIGMA BONDED TO CATION 5
:1 4 6 0
LIST THE CATIONS SIGMA BONDED TO CATION 6
:5 7 0
LIST THE CATIONS SIGMA BONDED TO CATION 7
:6 8 0
LIST THE CATIONS SIGMA BONDED TO CATION 8
:7 9 0
LIST THE CATIONS SIGMA BONDED TO CATION 9
:8 10 0
LIST THE CATIONS SIGMA BONDED TO CATION 10
:1 9 0




ENTER THE NUMBER OF THE CATION WHICH IS THE HETERO ATOM. IF THERE IS NO HETERO ATOM, ENTER ZERO.
:0
IF YOU DO NOT WISH TO SEE THE HAMILTONIAN TYPE SKIP
:

HAMILTONIAN REPRESENTATION

| | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|
| ALPHA | BETA | 0.0 | 0.0 | BETA | 0.0 | 0.C | 0.0 | 0.0 | BETA |
| BETA | ALPHA | BETA | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 |
| 0.0 | BETA | ALPHA | BETA | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 |
| 0.0 | 0.0 | BETA | ALPHA | BETA | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 |
| BETA | 0.0 | 0.0 | BETA | ALPHA | BETA | 0.0 | 0.0 | 0.0 | 0.0 |
| 0.0 | 0.0 | 0.0 | 0.0 | BETA | ALPHA | BETA | 0.0 | 0.0 | 0.0 |
| 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | BETA | ALPHA | BETA | 0.0 | 0.0 |
| 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | BETA | ALPHA | BETA | 0.0 |
| 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | BETA | ALPHA | BETA |
| BETA | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | BETA | ALPHA |

ENTER THE NUMBER OF PI ELECTRONS.
:10

NUMBER OF PI ELECTRONS 10
THERE IS NO HETEROATOM IN THE SIGMA FRAME

| ORBITAL ENERGIES IN ASCENDING ORDER | | | | OCCUPATION NUMBERS |
|---|---|---|---|---|
| E= ALPHA + | ( | 2.3102768E+00 | BETA ) | 2.00 |
| E= ALPHA + | ( | 1.6515723E+00 | BETA ) | 2.00 |
| E= ALPHA + | ( | 1.3556743E+00 | BETA ) | 2.00 |
| E= ALPHA + | ( | 8.8697524E-01 | BETA ) | 2.00 |
| E= ALPHA + | ( | 4.7726000E-01 | BETA ) | 2.00 |
| E= ALPHA + | ( | -4.0039232E-01 | BETA ) | 0.00 |
| E= ALPHA + | ( | -7.3764031E-01 | BETA ) | 0.00 |
| E= ALPHA + | ( | -1.5792181E+00 | BETA ) | 0.00 |
| E= ALPHA + | ( | -1.8692140E+00 | BETA ) | 0.00 |
| E= ALPHA + | ( | -2.0952940E+00 | BETA ) | 0.00 |

IF YOU DO NOT WISH TO SEE THE EIGENVECTORS
TYPE SKIP
:SKIP

GROUND STATE ENERGY 1.33635174E+01

LOWEST FREQUENCY OF ELECTRONIC SPECTRUM (IN UNITS OF BETA/H)
8.77652E-01

:

PI ELECTRON CHARGE DENSITIES

| | | | |
|---|---|---|---|
| ATOM NUMBER | 1 | CHARGE DENSITY | 1.02743E+00 |
| ATOM NUMBER | 2 | CHARGE DENSITY | 1.17288E+00 |
| ATOM NUMBER | 3 | CHARGE DENSITY | 1.04660E+00 |
| ATOM NUMBER | 4 | CHARGE DENSITY | 1.17288E+00 |
| ATOM NUMBER | 5 | CHARGE DENSITY | 1.02743E+00 |
| ATOM NUMBER | 6 | CHARGE DENSITY | 8.54946E-01 |
| ATOM NUMBER | 7 | CHARGE DENSITY | 9.86447E-01 |
| ATOM NUMBER | 8 | CHARGE DENSITY | 8.70001E-01 |
| ATOM NUMBER | 9 | CHARGE DENSITY | 9.86447E-01 |
| ATOM NUMBER | 10 | CHARGE DENSITY | 8.54946E-01 |

:

PI BOND ORDERS

| | | | | | | |
|---|---|---|---|---|---|---|
| BETWEEN ATOMS | 1 | AND | 2 | PI BOND ORDER IS | | 5.95632E-01 |
| BETWEEN ATOMS | 1 | AND | 5 | PI BOND ORDER IS | | 4.00945E-01 |
| BETWEEN ATOMS | 1 | AND | 10 | PI BOND ORDER IS | | 5.85798E-01 |
| BETWEEN ATOMS | 2 | AND | 3 | PI BOND ORDER IS | | 6.56039E-01 |
| BETWEEN ATOMS | 3 | AND | 4 | PI BOND ORDER IS | | 6.56039E-01 |
| BETWEEN ATOMS | 4 | AND | 5 | PI BOND ORDER IS | | 5.95632E-01 |
| BETWEEN ATOMS | 5 | AND | 6 | PI BOND ORDER IS | | 5.85798E-01 |
| BETWEEN ATOMS | 6 | AND | 7 | PI BOND ORDER IS | | 6.64039E-01 |
| BETWEEN ATOMS | 7 | AND | 8 | PI BOND ORDER IS | | 6.38899E-01 |
| BETWEEN ATOMS | 8 | AND | 9 | PI BOND ORDER IS | | 6.38899E-01 |
| BETWEEN ATOMS | 9 | AND | 10 | PI BOND ORDER IS | | 6.64039E-01 |